

Invariant closures for the Fokker–Planck equation

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We develop the principle of dynamic invariance to obtain closed moment equations from the Fokker–Planck kinetic equation. The analysis is carried out to explicit formulae for computation of the lowest eigenvalue and of the corresponding eigenfunction for arbitrary potentials.

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The Fokker–Planck equation (FPE) is a familiar model in various problems of nonequilibrium statistical physics [1]. In this paper we consider the FPE of the form

$$\partial_t W = \partial_x \cdot \{D \cdot [W \partial_x U + \partial_x W]\}. \quad (1)$$

Here $W(x, t)$ is the probability density over the configuration space x , at the time t , while $U(x)$ and $D(x)$ are the potential and the positively semi-definite ($y \cdot D \cdot y \geq 0$) diffusion matrix. The dot denotes convolution in the configuration space. The FPE (1) is particularly important in studies of polymer solutions [2]. Let us recall the two properties of the FPE (1), important to what will follow: (i). Conservation of the total probability: $\int W(x, t) dx = 1$. (ii). Dissipation: The equilibrium distribution, $W_{eq} \propto \exp(-U)$, is the unique stationary solution to the FPE (1). The entropy,

$$S[W] = - \int W(x, t) \ln \left[\frac{W(x, t)}{W_{eq}(x)} \right] dx, \quad (2)$$

is a monotonically growing function due to the FPE (1), and it arrives at the global maximum in the equilibrium. These properties are most apparent when the FPE (1) is rewritten as follows:

$$\partial_t W(x, t) = \hat{M}_W \frac{\delta S[W]}{\delta W(x, t)}, \quad (3)$$

where $\hat{M}_W = -\partial_x \cdot [W(x, t) D(x) \cdot \partial_x]$ is a positive semi-definite symmetric operator with kernel 1. The form (3) (the dissipative vector field is a metric transform of the entropy gradient) is an example of the dissipative part of a structure termed GENERIC in a recent series of papers [3].

Usually one is interested in dynamics of moments of the distribution function W rather than in the dynamics of the W itself. Except for simplest potentials U and diffusion matrices D , the moment equations, as they follow from the FPE (1), are not closed. Therefore, closure procedures are required.

In this paper we address the problem of closure for the FPE (1) in a general setting. First, we review the maximum entropy principle (MEP) as a source of suitable initial approximations for the closures. We also discuss a version of the MEP, valid for a near-equilibrium dynamics, and which results in explicit formulae for arbitrary U and D .

The MEP closures are almost never invariants of the true moment dynamics, and corrections to the MEP closures is the central issue of this paper. For this purpose, we apply the method of invariant manifold [4], which is carried out (subject to certain approximations explained below) to explicit recurrence formulae for one-moment near-equilibrium closures for arbitrary U and D . These formulae give a method for computing the lowest eigenvalue of the problem, and which dominates the near-equilibrium FPE dynamics.

MEP closures [5]. Let $M = \{M_0, M_1, \dots, M_k\}$ be linearly independent moments of interest, $M_i[W] = \int m_i(x) W(x) dx$, and where $m_0 = 1$. We assume existence a function $W^*(M, x)$ which extremizes the entropy S (2) under the constraints of fixed M . This MEP distribution function may be written

$$W^* = W_{eq} \exp \left[\sum_{i=0}^k \Lambda_i m_i(x) - 1 \right],$$

where $\Lambda = \{\Lambda_0, \Lambda_1, \dots, \Lambda_k\}$ are Lagrange multipliers. Closed equations for moments M are derived in two steps. First, the MEP distribution is substituted into the FPE (1) or (3) to give a formal expression: $\partial_t W^* = \hat{M}_{W^*}(\delta S / \delta W)|_{W=W^*}$. Second, applying a projector Π^* ,

$$\Pi^* \bullet = \sum_{i=0}^k (\partial W^* / \partial M_i) \int m_i(x) \bullet dx,$$

on both sides of this formal expression, we derive closed equations for M in the MEP approximation. Further processing requires an explicit solution to the constraints, $\int W^*(\Lambda, x) m_i(x) dx = M_i$, to get the dependence of Lagrange multipliers Λ on the moments M . Though typically the functions $\Lambda(M)$ are not known explicitly, one general remark about the moment equations is readily available. Specifically, the moment equations in the MEP approximation have the form:

$$\dot{M}_i = \sum_{j=0}^k M_{ij}^*(M) \frac{\partial S^*(M)}{\partial M_j}, \quad (4)$$

where $S^*(M) = S[W^*(M)]$ is the macroscopic entropy, and where M_{ij}^* is an M -dependent $(k+1) \times (k+1)$ matrix:

$$M_{ij}^* = \int W^*(M, x) [\partial_x m_i(x)] \cdot D(x) \cdot [\partial_x m_j(x)] dx.$$

The matrix M_{ij}^* is symmetric, positive semi-definite, and its kernel is the vector δ_{0i} . Thus, *the MEP closure reproduces the GENERIC structure on the macroscopic level*, the vector field of macroscopic equations (4) is a metric transform of the gradient of the macroscopic entropy.

Triangle MEP closures [6]. The following version of the MEP makes it possible to derive more explicit results in a general setting: In many cases, one can split the set of moments M in two parts, $M_I = \{M_0, M_1, \dots, M_l\}$ and $M_{II} = \{M_{l+1}, \dots, M_k\}$, in such a way that the MEP distribution can be constructed explicitly for M_I as $W_I^*(M_I, x)$. The full MEP problem for $M = \{M_I, M_{II}\}$ in the "shifted" formulation reads: extremize the functional $S[W_I^* + \Delta W]$ with respect to ΔW , subject to the constraints $M_I[W_I^* + \Delta W] = M_I$ and $M_{II}[W_I^* + \Delta W] = M_{II}$. Let us denote as ΔM_{II} deviations of the moments M_{II} from their values in the state W_I^* . For small deviations, the entropy is well approximated with a quadratic functional $\Delta S[\Delta W]$ which is an expansion of the functional (2) in the state W_I^* up to the terms of the order ΔW^2 . With $M_I[W_I^*] = M_I$, we come to the following problem: extremize the functional $\Delta S[\Delta W]$, subject to the constraints $M_I[\Delta W] = 0$, and $M_{II}[\Delta W] = \Delta M_{II}$. The solution to the latter problem is always explicitly found from a $(k+1) \times (k+1)$ system of linear algebraic equations for Lagrange multipliers.

In the remainder of this paper we deal with one-moment near-equilibrium closures: $M_I = M_0$, (i. e. $W_I^* = W_{eq}$), and the set M_{II} contains a single moment $M = \int m W dx$, $m(x) \neq 1$. We will specify notations for the near-equilibrium FPE, writing the distribution function as $W = W_{eq}(1 + \Psi)$, where the function Ψ satisfies an equation:

$$\partial_t \Psi = W_{eq}^{-1} \hat{J} \Psi, \quad (5)$$

where $\hat{J} = \partial_x \cdot [W_{eq} D \cdot \partial_x]$. The triangle one-moment MEP function reads:

$$W^{(0)} = W_{eq} \left[1 + \Delta M m^{(0)} \right] \quad (6)$$

where $\Delta M = M - \langle m \rangle$, and

$$m^{(0)} = [\langle mm \rangle - \langle m \rangle^2]^{-1} [m - \langle m \rangle]. \quad (7)$$

Brackets $\langle \dots \rangle = \int W_{eq} \dots dx$ denote equilibrium averaging. The superscript (0) indicates that the triangle MEP function (6) will be considered as an initial approximation to a procedure which we address below. Projector for the approximation (6) has the form

$$\Pi^{(0)} \bullet = W_{eq} \frac{m^{(0)}}{\langle m^{(0)} m^{(0)} \rangle} \int m^{(0)} \bullet dx. \quad (8)$$

substituting the function (6) into the FPE (5), and applying the projector (8) on both the sides of the resulting formal expression, we derive an equation for M : $\dot{M} = -\lambda_0 \Delta M$, where $1/\lambda_0$ is the inverse effective time of relaxation of the moment M to its equilibrium value, in the MEP approximation (6):

$$\lambda_0 = \langle m^{(0)} m^{(0)} \rangle^{-1} \langle \partial_x m^{(0)} \cdot D \cdot \partial_x m^{(0)} \rangle. \quad (9)$$

Invariant closures. Both the MEP and the triangle MEP closures are almost never invariants of the FPE dynamics. That is, the moments M of solutions to the FPE (1) vary in time differently from the solutions to the closed moment equations like (4), and these variations are generally significant even for the near-equilibrium dynamics. Therefore, we ask for corrections to the MEP closures to finish with the invariant closures [4].

First, the invariant one-moment closure is given by an unknown distribution function $W^{(\infty)} = W_{eq}[1 + \Delta M m^{(\infty)}(x)]$ which satisfies an equation

$$[1 - \Pi^{(\infty)}]\hat{J}m^{(\infty)} = 0. \quad (10)$$

Here $\Pi^{(\infty)}$ is a projector, associated with an unknown function $m^{(\infty)}$, and which is also yet unknown. Eq. (10) is a formal expression of the invariance principle for a one-moment near-equilibrium closure: considering $W^{(\infty)}$ as a manifold in the space of distribution functions, parameterized with the values of the moment M , we require that the microscopic vector field $\hat{J}m^{(\infty)}$ be equal to its projection, $\Pi^{(\infty)}\hat{J}m^{(\infty)}$, onto the tangent space of the manifold $W^{(\infty)}$.

Now we turn our attention to solving the invariance equation (10) iteratively, beginning with the triangle one-moment MEP approximation $W^{(0)}$ (6). We apply the following iteration process to the Eq. (10):

$$[1 - \Pi^{(k)}]\hat{J}m^{(k+1)} = 0, \quad (11)$$

where $k = 0, 1, \dots$, and where $m^{(k+1)} = m^{(k)} + \mu^{(k+1)}$, and the correction satisfies the condition $\langle \mu^{(k+1)} m^{(k)} \rangle = 0$. Projector is updated after each iteration, and it has the form

$$\Pi^{(k+1)} \bullet = W_{eq} \frac{m^{(k+1)}}{\langle m^{(k+1)} m^{(k+1)} \rangle} \int m^{(k+1)}(x) \bullet dx. \quad (12)$$

Applying $\Pi^{(k+1)}$ to the formal expression, $W_{eq} m^{(k+1)} \dot{M} = \Delta M [1 - \Pi^{(k+1)}] \hat{J}m^{(k+1)}$, we derive the macroscopic equation, $\dot{M} = -\lambda_{k+1} \Delta M$, where λ_{k+1} is the $(k+1)$ th update of the inverse effective time (9):

$$\lambda_{k+1} = \frac{\langle \partial_x m^{(k+1)} \cdot D \cdot \partial_x m^{(k+1)} \rangle}{\langle m^{(k+1)} m^{(k+1)} \rangle}. \quad (13)$$

Specializing to the one-moment near-equilibrium closures, and following a general argument [4], solutions to the invariance equation (10) are eigenfunctions of the operator \hat{J} , while the formal limit of the iteration process (11) is the eigenfunction which corresponds to the eigenvalue with the minimal nonzero absolute value.

Diagonal approximation. To obtain more explicit results in the iteration process (11), we introduce an approximate solution *on each iteration*. The correction $\mu^{(k+1)}$ satisfies the condition $\langle m^{(k)} \mu^{(k+1)} \rangle = 0$, and can be decomposed as follows: $\mu^{(k+1)} = \alpha_k e^{(k)} + e_{ort}^{(k)}$. Here $e^{(k)} = W_{eq}^{-1} [1 - \Pi^{(k)}] \hat{J}m^{(k)} = \lambda_k m^{(k)} + R^{(k)}$ is the variance of the k th approximation, where

$$R^{(k)} = \partial_x \cdot [D \cdot \partial_x m^{(k)}] - \partial_x U \cdot D \cdot \partial_x m^{(k)}. \quad (14)$$

The function $e_{ort}^{(k)}$ is orthogonal to both $e^{(k)}$ and $m^{(k)}$: $\langle e^{(k)} e_{ort}^{(k)} \rangle = 0$, and $\langle m^{(k)} e_{ort}^{(k)} \rangle = 0$. Our diagonal approximation (DA) consists in disregarding the part $e_{ort}^{(k)}$. Specifically, we consider the following ansatz at the k th iteration:

$$m^{(k+1)} = m^{(k)} + \alpha_k e^{(k)}. \quad (15)$$

Substituting the ansatz (15) into the Eq. (11), and integrating the latter expression with the function $e^{(k)}$, we evaluate the coefficient α_k :

$$\alpha_k = \frac{A_k - \lambda_k^2}{\lambda_k^3 - 2\lambda_k A_k + B_k}, \quad (16)$$

where parameters A_k and B_k represent the following equilibrium averages:

$$\begin{aligned} A_k &= \langle m^{(k)} m^{(k)} \rangle^{-1} \langle R^{(k)} R^{(k)} \rangle \\ B_k &= \langle m^{(k)} m^{(k)} \rangle^{-1} \langle \partial_x R^{(k)} \cdot D \cdot \partial_x R^{(k)} \rangle. \end{aligned} \quad (17)$$

Finally, putting together Eqs. (13), (14), (15), (16), and (17), we arrive at the following DA recurrency solution, and which is our main result:

$$m^{(k+1)} = m^{(k)} + \alpha_k [\lambda_k m^{(k)} + R^{(k)}], \quad (18a)$$

$$\lambda_{k+1} = \frac{\lambda_k - (A_k - \lambda_k^2) \alpha_k}{1 + (A_k - \lambda_k^2) \alpha_k^2}. \quad (18b)$$

To test the convergency of the DA process (18) we have considered two potentials U in the FPE (1) with a constant diffusion matrix D . The first test was with the square potential $U = x^2/2$, in the three-dimensional configuration space, since for this potential the detail structure of the spectrum is well known. We have considered two examples of initial one-moment MEP closures with $m^{(0)} = x_1 + 100(x^2 - 3)$ (example 1), and

$m^{(0)} = x_1 + 100x^6x_2$ (example 2), in the Eq. (7). The result of performance of the DA for λ_k (18b) is presented in the Table I, together with the error δ_k which was estimated as the norm of the variance at each iteration: $\delta_k = \langle e^{(k)} e^{(k)} \rangle / \langle m^{(k)} m^{(k)} \rangle$. In both examples, we see a good monotonic convergency to the minimal eigenvalue $\lambda_\infty = 1$, corresponding to the eigenfunction x_1 . This convergency is even striking in the example 1, where the initial choice was very close to a different eigenfunction $x^2 - 3$, and which can be seen in the non-monotonic behavior of the variance. Thus, we have an example to trust the DA as converging to the stationary point of the original iteration procedure (11).

For the second test, we have taken a one-dimensional potential $U = -50 \ln(1 - x^2)$, the configuration space is the segment $|x| \leq 1$. Potentials of this type (so-called FENE potential) are used in applications of the FPE to models of polymer solutions [2]. Results are given in the Table II for the two initial functions, $m^{(0)} = x^2 + 10x^4 - \langle x^2 + 10x^4 \rangle$ (example 3), and $m^{(0)} = x^2 + 10x^8 - \langle x^2 + 10x^8 \rangle$ (example 4). Both the examples demonstrate a stabilization of the λ_k at the same value after some ten iterations.

In conclusion, we have developed the principle of invariance to obtain moment closures for the Fokker-Planck equation (1), and have derived explicit results for the one-moment near-equilibrium closures, particularly important to get information about the spectrum of the FP operator.

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TABLE I. Iterations λ_k and the error δ_k for $U = x^2/2$.

		0	1	4	8	12	16	20
Ex. 1	λ	1.99998	1.99993	1.99575	1.47795	1.00356	1.00001	1.00000
	δ	$0.16 \cdot 10^{-4}$	$0.66 \cdot 10^{-4}$	$0.42 \cdot 10^{-2}$	0.24	$0.35 \cdot 10^{-2}$	$0.13 \cdot 10^{-4}$	$0.54 \cdot 10^{-7}$
Ex. 2		0	1	2	3	4	5	6
	λ	3.399	2.437	1.586	1.088	1.010	1.001	1.0002
	δ	1.99	1.42	0.83	0.16	$0.29 \cdot 10^{-1}$	$0.27 \cdot 10^{-2}$	$0.57 \cdot 10^{-3}$

TABLE II. Iterations λ_k for $U = -50 \ln(1 - x^2)$.

		0	1	2	3	4	5	6	7	8
Ex. 3	λ	213.1774	212.1864	211.9148	211.8619	211.8499	211.8453	211.8433	211.8422	211.8417
Ex. 4	λ	216.5856	213.1350	212.2123	211.9984	211.9295	211.8989	211.8838	211.8757	211.8713